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Optical Phonons and Electronic Properties in Double Heterostructures

by

D. L. Lin, R. Chen and Thomas F. George

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Optical phonons and electronic properties in double heterostructures

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ABSTRACT

Optical phonon modes in a semiconductor double heterostructure (DHS) are examined within the continuum model. The interface modes found here can account for the novel phenomena observed in right-angle Raman scattering. The Hamiltonian for the electron interaction with phonon eigenmodes is derived and employed to study polaronic effects in the DHS. The $1s$-$2p_+$ transition energy of a magnetopolaron bound to a hydrogenic impurity in the quantum well is calculated, and excellent agreement with experiments is obtained.

1. INTRODUCTION

It is by now well known that in polar crystals such as III-V compounds, the electron-optical-phonon interaction plays an important role in determining the electronic properties at higher temperatures. Since these compounds are the usual materials used in the fabrication of microstructures such as heterostructures and superlattices, there has been growing interest in the study of electron-phonon interactions in these structures. Until recently, the bulk Fröhlich Hamiltonian has been employed in almost all calculations, even though the presence of surfaces and interfaces is expected to change the nature of lattice vibration modes dramatically.[1,2]

Although surface optical (SO) phonon modes have been discussed some time ago,[3,4] they have not been included until fairly recently in the treatment of polarons confined in a slab[5] or near the interface in semi-infinite systems.[6,7] In recent papers,[8,9] the optical phonon modes in a double heterostructure (DHS) of polar crystals have been solved within the continuum model. It is found that there are only two types of phonon modes: the interface (IN) and the confined bulk modes. The latter may be either longitudinal (LO) or transversal (TO) phonon modes. Therefore, the Fröhlich Hamiltonian involving only the bulk LO phonon cannot be applied to quantum wells and other microstructures.

We report in this paper the Hamiltonian derived for the electron-optical-phonon interaction in a DHS. Both the interface and bulk LO phonons are included. The interaction Hamiltonian is then employed to study the phonon effects on electronic and optical properties in the DHS. The self-energy of a free polaron is calculated for arbitrary well width. It approaches the bulk value of the side material in the limit of $d \to 0$, and that of the central layer in the limit of $d \to \infty$. For a magnetopolaron bound to a hydrogenic impurity in the GaAs/AlGaAs quantum well, the transition energy calculated from this Hamiltonian exhibits the strange pinning phenomena in strong magnetic fields as observed experimentally.

2. OPTICAL PHONON MODES

The detailed solution of phonon eigenmodes can be found in Refs. 8 and 9. Here we just outline what is essential for our discussion of polaronic effects. The geometry of our DHS is shown in Fig. 1. Material ν ($\nu = 1,2$) is characterized by the dielectric constants $\epsilon_\nu(\omega)$, $\epsilon_{o\nu}$ and $\epsilon_{o\infty}$, plasma frequency $\omega_{p\nu}$, number of ion pairs n_ν per unit cell, natural frequency $\omega_{o\nu}$, and polarizability α_ν. The polarization vector $\vec{P}$ is related to the relative displacement $\vec{u}(\vec{r})$ of the ion pair and to the macroscopic field $\vec{E}$

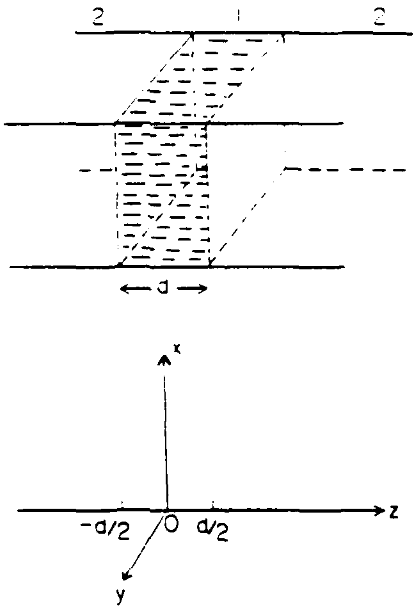

Figure 1. Geometry of the double heterostructure.

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$$\vec{p}(\vec{r}) = n_\nu e^*_\nu \eta_\nu^{-1/2}\, \vec{u}(\vec{r})$$

$$= \frac{1}{4\pi}\, \chi_\nu(\omega)\vec{E} \quad , \qquad (1)$$

where we have defined $\eta_\nu^{1/2} = [1 + \alpha_\nu n_\nu(\lambda_{o\nu} - \lambda_\nu)]^{-1}$ and

$$\lambda_{o\nu} = 4\pi\omega_{o\nu}^2/\omega_{p\nu}^2 \qquad \lambda_\nu = 4\pi\omega^2/\omega_{p\nu}^2 \quad . \qquad (2a,b)$$

The dielectric susceptibility $\chi_\nu(\omega)$ is given by

$$4\pi\chi_\nu^{-1} = (\lambda_{o\nu}-\lambda_\nu)\eta_\nu^{1/2} - 4\pi/3 \qquad (3)$$

and is related to the dielectric function by $\chi_\nu(\omega) = \epsilon_\nu(\omega) - 1$. With the frequency parameters (2), we find from (3)

$$\epsilon_\nu(\omega) = \epsilon_{\infty\nu}(\omega_{L\nu}^2 - \omega^2)/(\omega_{T\nu}^2 - \omega^2) \qquad (4a)$$

$$\epsilon_{\infty\nu} = 1 + 4\pi n_\nu\alpha_\nu/(1 - \frac{4\pi}{3} n_\nu\alpha_\nu) \quad . \qquad (4b)$$

The electrostatic potential $\phi(\vec{r})$ that gives rise to the field $\vec{E}$ satisfies

$$\vec{E}(\vec{r}) = -\nabla\phi(\vec{r}) \quad . \qquad (5)$$

On the assumption that the dielectric function $\epsilon_\nu(\omega)$ does not depend upon the spatial coordinates within each layer, we have from (5) and $\nabla\cdot\vec{D} = 0$

$$\epsilon_\nu(\omega)\nabla^2\phi(\vec{r}) = 0 \quad . \qquad (6)$$

Since the DHS does not possess translational invariance in the z-direction, the two-dimensional (2D) vectors $\vec{\kappa}$ and $\vec{\rho}$ are introduced in the wave vector $\vec{k} = (\vec{\kappa},q)$ and in the position vector $\vec{r} = (\vec{\rho},z)$. The potential can then be written as

$$\phi(\vec{r}) = \int d\vec{\kappa}\ \phi(\vec{\kappa},z)e^{i\vec{\kappa}\cdot\vec{\rho}} \quad . \qquad (7)$$

Substituting (7) in (6), we find that the Fourier components of the potential satisfy the equation

$$\epsilon_\nu(\omega)\left(\frac{\partial^2}{\partial z^2} - \kappa^2\right)\phi(\vec{\kappa},z) = 0 \quad , \qquad (8)$$

which may be solved by assuming either

$$\epsilon_\nu(\omega) = 0 \quad , \quad \nu = 1,2 \qquad (9a)$$

or

$$\left(\frac{\partial^2}{\partial z^2} - \kappa^2\right)\phi(\vec{\kappa},z) = 0 \quad . \qquad (9b)$$

It is seen from (4a) that (9a) is satisfied by the LO frequencies $\omega^2 = \omega_{L\nu}^2$. Because $\omega_{L1} \neq \omega_{L2}$, the vibrations on both sides of the interface have different time dependences. The boundary conditions that both ϕ and the electric displacement D_z must be continuous across the interfaces then require the confinement of the LO modes. On the other hand, Eq. (9b) yields the interface modes of vibration. The polarization eigenvectors of all these modes as well as the dispersion relations have been worked out in Ref. 8. It is also shown there that the novel slab modes observed in right-angle Raman scattering[10] can be interpreted as the interface modes. As discussed in Ref. 8, in the vicinity of the center of the first Brillouin zone, the antisymmetric interface modes, which are predominantly transversal, oscillate at longitudinal frequency while the symmetric interface modes are longitudinal but oscillate at transversal frequency. Using Eqs. (8) and (9), we find after a straightforward calculation electrostatic potentials corresponding to these modes. Thus for the confined LO modes, the Fourier components of the potential are

$$\phi_m(\vec{\kappa},z) = 4\pi C_m(\vec{\kappa}) \begin{cases} \sin(m\pi z/d) & , \text{ for even } m \\ \cos(m\pi z/d) & , \text{ for odd } m \end{cases} \tag{10a}$$

with the normalization constant

$$|C_m(\kappa)| = \omega_{p\nu}\eta_\nu^{-1/2} \sqrt{2/d}\, [\kappa^2 + (m\pi/d)^2]^{-1/2} \quad . \tag{10b}$$

Corresponding to the interface modes, the potentials are

$$\phi_{sj}(\vec{\kappa}\cdot z) = \begin{cases} C_{sj} e^{-\kappa|z|} & , \quad |z| > d/2 \\ C_{sj}(1 + \epsilon_2/\epsilon_1) \cosh(\kappa z) & , \quad |z| < d/2 \end{cases} \tag{11a}$$

for the symmetric modes and

$$\phi_{aj}(\vec{\kappa}\cdot z) = \begin{cases} -C_{aj} \operatorname{sgn}(z)\, e^{-\kappa|z|} & , \quad |z| > d/2 \\ C_{aj}(1 + \epsilon_2/\epsilon_1) \sinh(\kappa z) & , \quad |z| < d/2 \end{cases} \tag{11b}$$

for the antisymmetric modes. The function sgn(z) = 1 for z > 0 and -1 for z < 0. The index j = 1,2 in Eq. (11) labels the two branches of the symmetric or antisymmetric interface modes which have the same normalization constant as discussed in Ref. 8. The normalization constants are given by

$$|C_{sj}(\vec{\kappa})| = \frac{4\pi}{\sqrt{A}} \quad \epsilon^{\kappa d/2} \Big/ \left\{ 2\kappa \left[\frac{\eta_1 \chi_1^2}{\omega_{p1}^2} \tan(\frac{\kappa d}{2}) + \frac{\eta_2 \chi_2^2}{\omega_{p2}^2} \right] \right\}^{1/2} \tag{12a}$$

$$|C_{aj}(\vec{\kappa})| = \frac{4\pi}{\sqrt{A}}\, e^{\kappa d/2}\sqrt{\tanh(\frac{\kappa d}{2})} \;/\; \left\{2\kappa\left[\frac{\eta_1\chi_1^2}{\omega_{p1}^2} + \frac{\eta_2\chi_2^2}{\omega_{p2}^2}\tanh(\frac{\kappa d}{2})\right]\right\}^{1/2} \quad . \tag{12b}$$

3. ELECTRON-PHONON INTERACTIONS

To derive the Hamiltonian operator, we start with the free polarization or the free phonon. In terms of the polarization vector $\vec{\pi}$ and its canonical conjugate $\dot{\vec{\pi}}$, we can write the Hamiltonian in the form

$$H_{ph} = \frac{1}{2}\sum_{\alpha}\int d\vec{r}\, \frac{4\pi\eta_{\nu}}{\omega_{p\nu}^2}\, [\dot{\pi}^*_{\alpha}(\vec{r})\dot{\pi}_{\alpha}(\vec{r}) + \omega^2\pi^*_{\alpha}(\vec{r})\pi_{\alpha}(\vec{r})] \quad . \tag{13}$$

$\vec{\pi}$ and $\dot{\vec{\pi}}$ can be regarded as quantum mechanical operators and can be expressed in terms of their Fourier components as

$$\begin{aligned}\vec{\pi}(\vec{r}) = &\sum_{\vec{\kappa},m} \sqrt{\hbar/8\pi A\omega_{L\nu}}\, [a_m(\vec{\kappa}) + a^{\dagger}_m(-\vec{\kappa})]\vec{\pi}_m(\vec{r}) \\ &+ \sum_{\vec{\kappa},j}\left\{\sqrt{\hbar/8\pi A\omega_{sj}(\vec{\kappa})}\, [a_{sj}(\vec{\kappa}) + a^{\dagger}_{sj}(-\kappa)]\vec{\pi}_{sj}(\vec{r})\right. \\ &\left. + \sqrt{\hbar/8\pi A\omega_{aj}(\vec{\kappa})}\, [a_{aj}(\vec{\kappa}) + a^{\dagger}_{aj}(-\vec{\kappa})]\vec{\pi}_{aj}(\vec{r})\right\}\end{aligned} \tag{14a}$$

$$\begin{aligned}\dot{\vec{\pi}}(\vec{r}) = &\sum_{\vec{\kappa},m} i\sqrt{\hbar\omega_{L\nu}/8\pi A}\, [a_m(\vec{\kappa}) - a^{\dagger}_m(\vec{\kappa})]\vec{\pi}_m(\vec{r}) \\ &+ \sum_{\vec{\kappa},j}\left\{i\sqrt{\hbar\omega_{sj}(\vec{\kappa})/8\pi A}\, [a_{sj}(\vec{\kappa}) - a^{\dagger}_{sj}(-\vec{\kappa})]\vec{\pi}_{sj}(\vec{r})\right. \\ &\left. + i\sqrt{\hbar\omega_{aj}(\vec{\kappa})/8\pi A}\, [a_{aj}(\vec{\kappa}) - a^{\dagger}_{aj}(-\vec{\kappa})]\, \vec{\pi}_{aj}(\vec{r})\right\} \quad .\end{aligned} \tag{14b}$$

In Equations (14), we have introduced the area A of the interface, and the creation (annihilation) operators $a^{\dagger}_m(\vec{\kappa})$ $(a_m(\vec{\kappa}))$ for the confined modes and $a^{\dagger}_{sj,aj}(\vec{\kappa})$ $(a_{sj,aj}(\vec{\kappa}))$ for the symmetric and antisymmetric interface modes of phonons. They obey the commutation relations

$$[a_\alpha(\vec{\kappa}), a_\beta^\dagger(\vec{\kappa}')] = \delta_{\alpha\beta}\,\delta(\vec{\kappa}-\vec{\kappa}') \tag{15a}$$

$$[a_\alpha^\dagger(\vec{\kappa}),\ a_\beta^\dagger(\vec{\kappa}')] = [a_\alpha(\vec{\kappa}), a_\beta(\vec{\kappa}')] = 0 \quad . \tag{15b}$$

Using these commutators as well as the orthonormality relation for the eigenvectors, it is straightforward to show that

$$H_{ph} = H_{LO} + H_{IN} \tag{16a}$$

$$H_{LO} = \sum_{\vec{\kappa},m} \hbar\omega_{L\nu}\ [a_m^\dagger(\vec{\kappa})a_m(\vec{\kappa}) + \frac{1}{2}] \tag{16b}$$

$$H_{IN} = \sum_{\vec{\kappa},j} \left\{\hbar\omega_{sj}(\vec{\kappa})[a_{sj}^\dagger(\vec{\kappa})\ a_{sj}(\vec{\kappa}) + \frac{1}{2}] + \hbar\omega_{aj}(\vec{\kappa})[a_{aj}^\dagger(\vec{\kappa})a_{aj}(\vec{\kappa}) + \frac{1}{2}]\right\} \quad . \tag{16c}$$

The interaction energy for an electron interacting with the polarization at a point $\vec{r}$ is represented by the Hamiltonian

$$H_{e\text{-}ph} = -\ e\phi(\vec{r}) \quad . \tag{17}$$

Regarded as a quantum mechanical operator, the scalar field can be expressed, with the help of (1), (4) and (5), as

$$\begin{aligned}\phi(\vec{r}) = &\sum_{\vec{\kappa},m} \sqrt{\hbar/8\pi A\omega_{L\nu}}\ [a_m(\vec{\kappa}) + a_m^\dagger(-\vec{\kappa})]\phi_m(\vec{r}) \\ &+ \sum_{\vec{\kappa},j} \left\{\sqrt{\hbar/8\pi A\omega_{sj}(\vec{\kappa})}\ [a_{sj}(\vec{\kappa}) + a_{sj}^\dagger(-\vec{\kappa})]\phi_{sj}(\vec{r})\right. \\ &\left.+ \sqrt{\hbar/8\pi A\omega_{aj}(\vec{\kappa})}\ [a_{aj}(\vec{\kappa}) + a_{aj}^\dagger(-\vec{\kappa})]\phi_{aj}(\vec{r})\right\} \quad .\end{aligned} \tag{18}$$

Combining (10a), (11) and (18), we find after some algebra the interaction Hamiltonian

$$H_{e\text{-}ph} = H_{e\text{-}LO} + H_{e\text{-}IN} \tag{19}$$

$$H_{e\text{-}LO} = -\sum_{\vec{\kappa}} e^{i\vec{\kappa}\cdot\vec{\rho}} \left\{\sum_{m=1,3\ldots} B_m(\kappa)\cos(\frac{m\pi z}{d})[\hat{a}_m(\vec{\kappa}) + \hat{a}_m^\dagger(-\vec{\kappa})]\right.$$

$$+ \sum_{m=2,4...} B_m(\kappa) \sin(\frac{m\pi z}{d})[\hat{a}_m(\vec{\kappa}) + \hat{a}_m^{\dagger}(-\vec{\kappa})]\Big\} \tag{20}$$

$$H_{e-IN} = - \sum_{\vec{\kappa},j} e^{i\vec{\kappa}\cdot\vec{\rho}-\kappa(|z|-d/2)} \Big\{B_{sj}(\vec{\kappa}) \; [\hat{a}_{s,j}(\vec{\kappa}) + \hat{a}_{s,j}^{\dagger}(-\vec{\kappa})]$$

$$- \operatorname{sgn}(z)B_{aj}(\kappa)[\hat{a}_{a,j}(\vec{\kappa}) + \hat{a}_{a,j}^{\dagger}(-\vec{\kappa})]\Big\} \qquad \text{for } |z| > d/2 \tag{21a}$$

$$H_{e-IN} = - \sum_{\vec{\kappa},j} e^{i\vec{\kappa}\cdot\vec{\rho}}\Big\{B_{sj}(\kappa) \; \frac{\cosh(\kappa z)}{\cosh(\kappa d/2)} \; [\hat{a}_{s,j}(\vec{\kappa}) + \hat{a}_{s,j}^{\dagger}(-\vec{\kappa})]$$

$$- B_{aj}(\kappa) \; \frac{\sinh(\kappa z)}{\sinh(\kappa d/2)} \; [\hat{a}_{a,j}(\vec{\kappa}) + \hat{a}_{a,j}^{\dagger}(-\vec{\kappa})]\Big\} \qquad \text{for } |z| < d/2 \quad . \tag{21b}$$

The coefficients can be calculated from (10b) and (12). The results are

$$|B_m(\vec{\kappa})|^2 = \frac{e^2\hbar}{8\pi A\omega_{L\nu}} \; |C_m(\vec{\kappa})|^2 = \frac{4\pi e^2\hbar\omega_{L\nu}}{Ad(\kappa^2 + \frac{m\pi}{d})} \left[\frac{1}{\epsilon_{\infty\nu}} - \frac{1}{\epsilon_{0\nu}}\right] \tag{22a}$$

$$|B_{sj,aj}(\vec{\kappa})|^2 = \frac{e^2\hbar}{8\pi A\omega_{sj,aj}(\vec{\kappa})} \; e^{-\kappa d} \; |C_{sj,aj}(\vec{\kappa})|^2 \quad , \tag{22b}$$

which leads to

$$|B_{sj}(\vec{\kappa})|^2 = \frac{\pi e^2}{A\kappa} - \hbar\omega_{sj}(\vec{\kappa})/[\bar{\epsilon}_1\tanh(\frac{\kappa d}{2}) + \bar{\epsilon}_2] \tag{23a}$$

$$|B_{aj}(\vec{\kappa})|^2 = \frac{\pi e^2}{A\kappa} - \hbar\omega_{aj}(\vec{\kappa})/[\bar{\epsilon}_1\coth(\frac{\kappa d}{2}) + \bar{\epsilon}_2] \quad . \tag{23b}$$

For convenience, we have defined in (23) the dielectric functions $\bar{\epsilon}_\nu(\omega)$ by

$$\frac{1}{\bar{\epsilon}_\nu(\omega)} = \frac{1}{\epsilon_\nu(\omega) - \epsilon_{0\nu}} - \frac{1}{\epsilon_\nu(\omega) - \epsilon_{\infty\nu}} \quad . \tag{24}$$

4. POLARON IN A DHS

We now proceed to calculate the polaron self-energy by perturbation theory. The unperturbed ground-state wave function is taken to be

$$|\psi_0\rangle = |\vec{k},0;\, n_{\vec{\kappa},\beta}\rangle = \frac{1}{\sqrt{A}}\, e^{i\vec{k}\cdot\vec{\rho}}\, f(z)\, |n_{\vec{\kappa},\beta}\rangle \quad , \qquad (25)$$

where electron states are characterized by a plane wave $\vec{k}$ in the xy-plane and the ground state 0 in the z-direction. The electron wave vector is defined as $\vec{k}_e = (\vec{k}, k_z)$ and the electron ground state wave function in a quantum well is given by

$$f(z) = \begin{cases} C\cos(k_z d/2)\exp[ik'_z(|z|-d/2)] \; , & |z| \geq d/2 \\ C\cos(k_z z) \; , \quad |z| < d/2 \end{cases} \quad . \qquad (26)$$

The wave numbers k_z and k'_z are related to the electron subband energy E_ℓ by

$$k_z = \sqrt{2m_e E_\ell/\hbar^2} \quad , \quad k'_z = \sqrt{2m_e(V_o - E_\ell)/\hbar^2} \qquad (27)$$

with E_ℓ determined by the transcendental equation

$$E_\ell = V_o \cos^2\left(\frac{d}{2}\sqrt{2m_e E_\ell/\hbar^2}\right) \quad , \quad \ell = 1, 2, \ldots \qquad (28)$$

The normalization constant C is given by

$$C = \sqrt{2k'_z/(k'_z d + 2)} \quad . \qquad (29)$$

The phonon state $|n_{\vec{k},\beta}\rangle$ is specified by n phonons with wave vector $\vec{k} = (\vec{\kappa}, q)$ and index β labeling the phonon mode, which may be one of the interface or confined LO modes.

The unperturbed energy of the electron in the ground state (25) can be written as

$$\epsilon^{(0)}_{\vec{k}_e} = \frac{\hbar k^2}{2m_e} + E_\ell + \sum_{\vec{\kappa},\beta} (n+\tfrac{1}{2})\, \hbar\omega_{\vec{\kappa},\beta} \quad . \qquad (30)$$

In the weak-coupling approximation, the corrections due to the electron-phonon interaction can be calculated by standard perturbation theory as

$$\epsilon_{\vec{k}_e} - \epsilon^{(0)}_{\vec{k}_e} = \sum_{\vec{\kappa},\beta} |\langle \vec{k}, 1_{\vec{\kappa},\beta}| H_{e\text{-}ph} |\vec{k}-\vec{\kappa}, 0_{\vec{\kappa},\beta}\rangle|^2 \Big/ \left(\epsilon^{(0)}_{\vec{k}} - \epsilon^{(0)}_{\vec{k}-\vec{\kappa}} - \hbar\omega_{\vec{\kappa},\beta}\right)$$

$$= \Delta E_1 + \Delta E_2 + \Delta E_3 \quad , \qquad (31)$$

where we have assumed that transistions to or from a state with more than one phonon are negligible. Because we are only interested in the electron self-energy due to electron-phonon interactions, matrix elements corresponding to interband transitions are all ignored. With the Hamiltonian operators given by (19)-(21), and the wave function by (25), we find, after integration over the phonon momentum, that

$$\Delta E_1 = -\alpha_{L1}\hbar\omega_{L1} - \gamma_{L1}\,\hbar^2 k/2m_e \qquad (32a)$$

$$\Delta E_2 = -\alpha_{L2}\hbar\omega_{L2} - \gamma_{L2}\,\hbar^2 k^2/2m_e \qquad (32b)$$

$$\Delta E_3 = -\sum_j \int_0^\infty d\kappa\; \alpha_{IN}(\kappa)\hbar\omega_{sj}(\kappa) - \gamma_{IN}\,\hbar^2 k^2/2m_e \quad . \qquad (32c)$$

The parameters α and γ are related to the Fröhlich-type coupling constants involving the particular phonon modes indicated by the subscripts. Explicitly, the α's are given by

$$\alpha_{L1} = \frac{4\alpha_{F1}}{K_{p1}d}\,|C|^4 \sum_{m=1,3\ldots} \left(\frac{d}{m\pi}\right)^2\left[1 + \frac{\cos(k_z d)}{1 - \left(\frac{2k_z d}{\mu\pi}\right)^2}\right]\left[\left(\frac{\pi}{K_{p1}d}\right)^2 - 1\right]^{-1} \ell n\left|\frac{m\pi}{K_{p1}d}\right| \qquad (33a)$$

$$\alpha_{L2} = \frac{4\alpha_{F2}}{\pi K_{p2}^2}\,|C|^4 \cos^4(k_z d/2) \int_0^\infty dt\, \frac{t^2 \ell n|t|}{[t^2 + 4(k_z'/K_{p2})^2]^2 (t^2 - 1)} \qquad (33b)$$

$$\alpha_{IN} = \alpha_{Fsj}(\kappa)\;|C|^4/K_{psj}(\kappa)Q^2(\kappa)\;\left[\left(\frac{\kappa}{K_{psj}(\kappa)}\right)^2 + 1\right] \quad , \qquad (33c)$$

and we have defined the function

$$Q^{-1}(\kappa) = \frac{2\cos^2(k_z d/2)}{\kappa + 2k_z'} + \frac{\tanh(\kappa d/2)}{\kappa} + \frac{2k_z \sin(k_z d)}{\kappa^2 + 4k_z^2}$$
$$+ \frac{\kappa}{\kappa^2 + 4k_z^2}\tanh\left(\frac{\kappa d}{2}\right)\cos(k_z d) \quad . \qquad (34)$$

K_{p1}^{-1} and K_{p2}^{-1} measure the polaron size due to the LO phonon in materials 1 and 2, respectively, while α_{F1} (α_{F2}) denotes the usual LO-phonon-electron coupling constant of the Frölich type in material 1 (2). They are given by

$$\gamma_{L1} = \frac{4\alpha_{F1}}{K_{p1}d} |C|^4 \sum_{m=1,3,\ldots} \left(\frac{d}{m\pi}\right)^2 \left[1 + \cos(k_z d)/[1 - \frac{2k_z d}{m\pi}]\right]^2$$

$$\times \int_0^\infty dt \; t/\left[t + \left(\frac{m\pi}{K_{p1}d}\right)^2\right](t+1)^3 \tag{35a}$$

$$\gamma_{L2} = \frac{\alpha_{F2}}{k_z' K_{p2}} \cos^4(k_z d/2) \int_0^\infty dt \; t/(\sqrt{t} + 2k_z'/K_{p2})^2 (t+1)^3 \tag{35b}$$

$$\gamma_{IN} = \sum_j \int_0^\infty d\kappa \; 2\kappa^2 \alpha_{Fsj}(\kappa)|C|^4/K_{psj}^3 Q^2(\kappa)[(\kappa/K_{psj})^2 + 1]^3 \quad . \tag{35c}$$

Substituting Eqs. (32) into (31) we find

$$\epsilon_{\vec{k}_e} - \epsilon_{\vec{k}_e}^{(0)} = -\alpha_{L1}\hbar\omega_{L1} - \alpha_{L2}\hbar\omega_{L2} - \sum_j \int_0^\infty d\kappa \; \alpha_{IN}(\kappa)\hbar\omega_{sj}(\kappa)$$

$$- \frac{\hbar^2 k^2}{2m_e}(\gamma_{L1} + \gamma_{L2} + \gamma_{IN}) \quad . \tag{36}$$

Combining (36) and the unperturbed energy (30), we obtain immediately the ground-state energy of the interacting electron-phonon system as

$$\epsilon_{\vec{k}_e} = \frac{\hbar^2 k^2}{2m_e^*} + E_\ell + \sum_{\vec{\kappa},\beta} (n + \frac{1}{2}) \hbar\omega_{\kappa,\beta} - \Delta E \quad , \tag{37}$$

where

$$m_e^* = m_e/(1 - \gamma_{L1} - \gamma_{L2} - \gamma_{IN}) \tag{38}$$

is the polaron effective mass and

$$\Delta E = \alpha_{L1}\hbar\omega_{L1} + \alpha_{L2}\hbar\omega_{L2} + \sum_j \int_0^\infty d\kappa \; \alpha_{IN}(\kappa)\hbar\omega_{sj}(\kappa) \tag{39}$$

Equation (39) is now employed to compute the binding energy of a polaron in the GaAs quantum well of a GaAs/AℓAs double heterostructure. The results are plotted as a function of the well width d in Fig. 2 in which contributions from the confined LO modes and interface modes are shown by dotted and dashed lines, respectively.

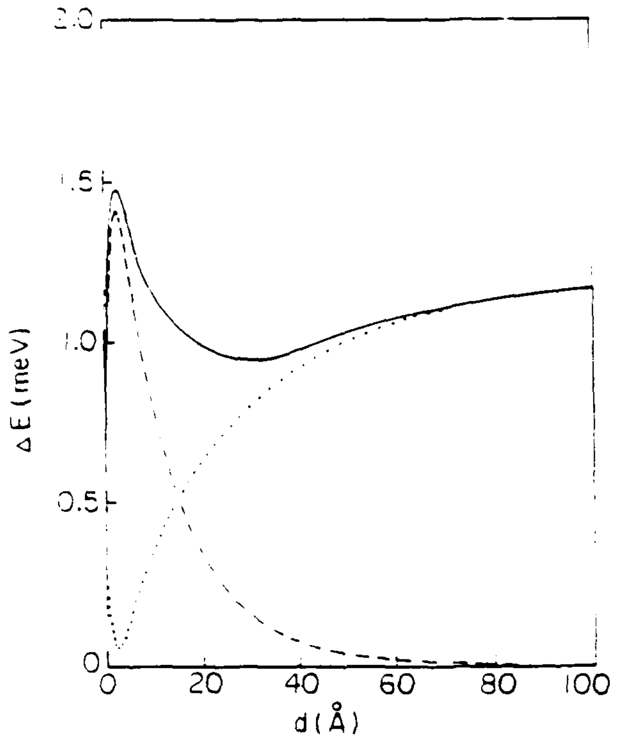

Figure 2. Polaron binding energy as a function of the well width. The dotted and dashed lines represent the contributions from confined LO and interface modes, respectively.

It is observed that for small d, our results are qualitatively different from what can be found in the literature. In fact, this is the first calculation that gives in the limit of $d \to 0$ the correct self-energy , the corresponding value in material 2. This is because we have included the contribution from confined LO phonons in material 2 in our Hamiltonian. The interface modes play an important role in the small-d regime. Their influence quickly diminishes as d increases. It is important to note that interface phonons are responsible for the pinning effect observed in a quantum well on the transition energy of the polaron bound to a hydrogenic impurity.[11] This is discussed in the following section.

5. TRANSITION ENERGY OF A BOUND MAGNETOPOLARON

Recent experiments[11,12] reveal that the resonant effect of the electron-phonon-interaction on the 1s-2p transition energy of a magnetopolaron bound to a hydrogenic impurity in GaAs/AlGaAs multiple-quantum-well structures exhibits the pinning phenomenon at an energy below the TO-phonon energy. To our knowledge, the origin of this surprising effect has not been understood.[13] Here we attempt to calculate this transition energy in the GaAs well of a GaAs/AlGaAs DHS.

Consider a donor impurity at the center of the well as in the case of the sample used in the experiments. A magnetic field is applied along the axis of the quantum well. The total Hamiltonian can be written as

$$H = H_e + H_{ph} + H_{e\text{-}ph} \quad , \tag{40}$$

where

$$H_e = [\vec{p} - \frac{e}{c}\vec{A}]/2m_e - \frac{e^2}{\epsilon_o r} + V_B(z) \tag{41a}$$

represents the energy of a hydrogenic impurity confined in the square well given by

$$V_B(z) = \begin{cases} 0 \quad , & |z| \leq d/2 \\ V_o \quad , & |z| > d/2 \end{cases} \quad , \tag{41b}$$

the free phonon energy H_{ph} is given by (16) and the interaction $H_{e\text{-}ph}$ by (19)-(21).

The unperturbed energy levels of the hydrogenic impurity described by (41a) are calculated variationally. For the trial wave function, we take

$$\psi = f(z)\ G(\rho,z,\phi) \quad . \tag{42}$$

The function f(z) is the solution to the square-well problem and is given by

$$f(z) = \begin{cases} \cos\ (k_z) \quad , & z \leq d/2 \\ \\ Ae^{-k'_z z} \quad , & z > d/2 \end{cases} \quad , \tag{43}$$

where k_z and k'_z are defined in (27) with E_ℓ representing the energy of the first subband. The function $G(\rho,z,\phi)$ describes the internal states of the donor and is chosen to reflect the symmetry properties of the system,

$$G(\rho,z,\phi) = \rho^{|m|}\ e^{im\phi}\ e^{-\gamma\rho^2/4}\ e^{-\gamma\xi^2 z^2/4} \quad , \tag{44}$$

where ξ is the variational parameter to be determined by minimizing the ground-state energy.

The interaction $H_{e\text{-}ph}$ is then treated as a perturbation, and the energy levels are calculated by means of Wigner-Brillouin perturbation theory. The result is[14]

$$\mathcal{E}_i(B) = E_i(B) + \frac{1}{(2\pi)^2} \sum_n \int d^2\kappa\ \frac{|\langle n|H_{e\text{-}ph}|i\rangle|^2}{\mathcal{E}_i(B) - E_n(B) - \hbar\omega(\vec{\kappa})} \quad , \tag{45}$$

where $E_i(B)$ stands for the corresponding unperturbed energy. The calculation is rather complicated, and detailed discussion of the procedures will be published elsewhere.[15] Here we just mention that the Hilbert space has been truncated to only the lowest three states in our second-order perturbation term. In other words, only 1s, $2p_+$ and $2p_-$ are included. For the particular samples used in these experiments,[11,12] all other states including $2p_0$ are pushed up by the quantum well way too high because of the broken symmetry and cannot be reached with presently-available magnetic fields. Furthermore, interactions of the electron with lattice vibrations outside the well under consideration are ignored, since they are important only for a very narrow ($d \lesssim 10$ Å) well, while d is larger than 100 Å in the experiments considered here.

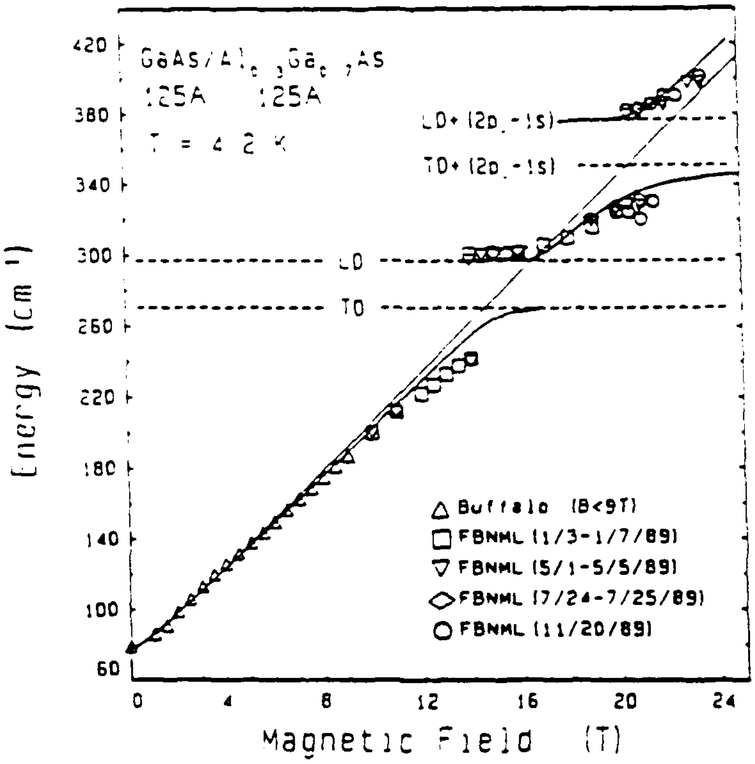

Figure 3. 1s-$2p_+$ transition energy as a function of the magnetic field B. Data are taken at SUNY-Buffalo and at the Francis Bitter National Magnet Laboratory in a series of measurements as indicated at the lower right corner. The heavy solid line represent results from the present theory and the straight line is the result without electron-phonon interaction.

The 1s-$2p_+$ transition energy calculated by computer iteration is plotted as a function of the field B in Fig. 3 along with the newly-improved set of data.[12] It is remarkable that the theoretical curve breaks into three branches separated by two gaps, in good agreement with experiments. The occurrence of gaps reflects the energy level repelling caused by the strong resonance interaction when the transition energy matches the phonon energy. Since the electron does not couple to TO-phonons, this pinning phenomenon must be due to the electron interaction with interface phonons which oscillate at frequencies between the bulk ω_L and ω_T. The interface-phonon coupling alone, however, is not adequate for a complete understanding of this phenomenon. There are still small discrepancies between experimental data and the theory, especially in the lower branch near the gap. Minor corrections such as the nonparabolic effect on the effective mass can probably account for the discrepancies. This and other possible corrections will be discussed in a forthcoming article.[15]

6. ACKNOWLEDGMENTS

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